What is claimed is:

1. A method for identifying a pharmacocluster, comprising:

(a) determining bound conformations of a ligand bound to different polypeptides; and

(b) clustering two or more bound conformations of said ligand having substantially the same bound conformation, thereby identifying a pharmacocluster.

2. The method of claim 1, wherein substantially the same bound conformation comprises a root mean square deviation of less than 1.1 Å.

3. The method of claim 1, wherein said ligand is selected from the group consisting of adenosine triphosphate, adenosine diphosphate, adenosine monophosphate thiamine (vitamin B_1), riboflavin (vitamin B_2), pyridoximine (vitamin B_6), cobalamin (vitamin B_{12}), pyrophosphate, flavin adenine dinucleotide (FAD), flavin mononucleotide (FMN), pyridoxal phosphate, coenzyme A, ascorbate (vitamin C), niacin, biotin, heme, porphyrin, folate, tetrahydrofolate, guanosine triphosphate, cytidine triphosphate, thymidine triphosphate, uridine triphosphate, retinol (vitamin A), calciferol (vitamin D_2), ubiquinone, ubiquitin, α-tocopherol (vitamin E), farnesyl, geranylgeranyl, pterin, pteridine or S-adenosyl methionine (SAM).

4. The method of claim 1, wherein said ligand comprises a nicotinamide adenine dinucleotide-related molecule.

5. The method of claim 4, wherein said nicotinamide adenine dinucleotide-related molecule is selected from the group consisting of oxidized nicotinamide adenine dinucleotide, reduced nicotinamide adenine dinucleotide, oxidized nicotinamide adenine dinucleotide phosphate, reduced nicotinamide adenine dinucleotide phosphate, and a mimetic thereof.

6. A method for identifying a member of a pharmacocluster, comprising:

(a) determining a bound conformation of a ligand bound to a polypeptide; and

(b) determining a pharmacocluster having substantially the same bound conformation as said bound conformation, thereby identifying said bound conformation of said ligand as a member of said pharmacocluster.

7. The method of claim 6, wherein substantially the same bound conformation comprises a root mean square deviation of less than 1.1 Å.

8. The method of claim 6, wherein said ligand is selected from the group consisting of adenosine triphosphate, adenosine diphosphate, adenosine monophosphate thiamine (vitamin B_1), riboflavin (vitamin B_2), pyridoximine (vitamin B_6), cobalamin (vitamin B_{12}), pyrophosphate, flavin adenine dinucleotide (FAD), flavin mononucleotide (FMN), pyridoxal phosphate, coenzyme A, ascorbate (vitamin C), niacin, biotin, heme, porphyrin, folate, tetrahydrofolate, guanosine triphosphate, cytidine triphosphate, thymidine triphosphate, uridine triphosphate, retinol (vitamin A), calciferol (vitamin D_2), ubiquinone, ubiquitin, α-tocopherol (vitamin E), farnesyl, geranylgeranyl, pterin, pteridine or S-adenosyl methionine (SAM).

9. The method of claim 6, wherein said ligand comprises a nicotinamide adenine dinucleotide-related molecule.

10. The method of claim 9, wherein said nicotinamide adenine dinucleotide-related molecule is selected from the group consisting of oxidized nicotinamide adenine dinucleotide, reduced nicotinamide adenine dinucleotide, oxidized nicotinamide adenine dinucleotide phosphate, reduced nicotinamide adenine dinucleotide phosphate, and a mimetic thereof.

11. A method for identifying a conformation-dependent property of a ligand, comprising:

(a) determining bound conformations of a ligand bound to different polypeptides;

(b) identifying two or more bound conformations of said ligand having substantially the same bound conformation; and

(c) identifying a conformation-dependent property of said bound conformations of said ligand having substantially the same bound conformation, said conformation-dependent property being correlated with said bound conformation of said ligand.

12. The method of claim 11, wherein said conformation-dependent property comprises a spectroscopic signal.

13. The method of claim 11, wherein said conformation-dependent property comprises an NMR signal.

14. The method of claim 13, wherein said NMR signal is selected from the group consisting of chemical shift, *J* coupling, dipolar coupling, cross-correlation, nuclear spin relaxation, transferred nuclear Overhauser effect, and any combination thereof.

15. The method of claim 11, wherein substantially the same bound conformation comprises a root mean square deviation of less than 1.1 Å.

16. The method of claim 11, wherein said ligand is selected from the group consisting of adenosine triphosphate, adenosine diphosphate, adenosine monophosphate thiamine (vitamin B_1), riboflavin (vitamin B_2), pyridoximine (vitamin B_6), cobalamin (vitamin B_{12}), pyrophosphate, flavin adenine dinucleotide (FAD), flavin mononucleotide (FMN), pyridoxal phosphate, coenzyme A, ascorbate (vitamin C), niacin, biotin, heme, porphyrin, folate, tetrahydrofolate, guanosine triphosphate, cytidine triphosphate, thymidine triphosphate, uridine triphosphate, retinol (vitamin A), calciferol (vitamin D_2), ubiquinone, ubiquitin, α-tocopherol (vitamin E), farnesyl, geranylgeranyl, pterin, pteridine or S-adenosyl methionine (SAM).

17. The method of claim 11, wherein said ligand comprises a nicotinamide adenine dinucleotide-related molecule.

18. The method of claim 17, wherein said nicotinamide adenine dinucleotide-related molecule is selected from the group consisting of oxidized nicotinamide adenine dinucleotide, reduced nicotinamide adenine dinucleotide, oxidized nicotinamide adenine dinucleotide phosphate, reduced nicotinamide adenine dinucleotide phosphate, and a mimetic thereof.

19. A method for identifying polypeptide pharmacofamilies, comprising:

(a) determining bound conformations of a ligand bound to different polypeptides of a polypeptide family; and

(b) identifying two or more bound conformations of said ligand having substantially different bound conformations, thereby identifying at least two polypeptide pharmacofamilies exhibiting binding specificity for said two or more substantially different bound conformations of said ligand.

20. The method of claim 19, wherein said polypeptide pharmacofamily is selected from the group consisting of pharmacofamily 1, pharmacofamily 2, pharmacofamily 3, pharmacofamily 4, pharmacofamily 5, pharmacofamily 6, pharmacofamily 7, and pharmacofamily 8.

21. The method of claim 19, wherein said ligand is selected from the group consisting of adenosine triphosphate, adenosine diphosphate, adenosine monophosphate thiamine (vitamin B_1), riboflavin (vitamin B_2), pyridoximine (vitamin B_6), cobalamin (vitamin B_{12}), pyrophosphate, flavin adenine dinucleotide (FAD), flavin mononucleotide (FMN), pyridoxal phosphate, coenzyme A, ascorbate (vitamin C), niacin, biotin, heme, porphyrin, folate, tetrahydrofolate, guanosine triphosphate, cytidine triphosphate, thymidine triphosphate, uridine triphosphate, retinol (vitamin A), calciferol (vitamin D_2), ubiquinone, ubiquitin, α-tocopherol (vitamin E), farnesyl, geranylgeranyl, pterin, pteridine or S-adenosyl methionine (SAM).

22. The method of claim 19, wherein said ligand comprises a nicotinamide adenine dinucleotide-related molecule.

23. The method of claim 22, wherein said nicotinamide adenine dinucleotide-related molecule is selected from the group consisting of oxidized nicotinamide adenine dinucleotide, reduced nicotinamide adenine dinucleotide, oxidized nicotinamide adenine dinucleotide phosphate, reduced nicotinamide adenine dinucleotide phosphate, and a mimetic thereof.

24. A method for identifying a member of a polypeptide pharmacofamily, comprising:

(a) determining a conformation-dependent property of a ligand bound to a polypeptide; and

(b) determining a pharmacocluster having substantially the same conformation-dependent property as said conformation-dependent property determined for said bound ligand, wherein a polypeptide pharmacofamily binds said ligand in a conformation of said pharmacocluster, thereby identifying said polypeptide as a member of said polypeptide pharmacofamily.

25. The method of claim 24, wherein said conformation-dependent property comprises a spectroscopic signal.

26. The method of claim 24, wherein said conformation-dependent property comprises an NMR signal.

27. The method of claim 26, wherein said NMR signal is selected from the group consisting of chemical shift, *J* coupling, dipolar coupling, cross-correlation, nuclear spin relaxation, transferred nuclear Overhauser effect, and any combination thereof.

28. The method of claim 24, wherein said ligand is selected from the group consisting of adenosine triphosphate, adenosine diphosphate, adenosine monophosphate thiamine (vitamin B_1), riboflavin (vitamin B_2), pyridoximine (vitamin B_6), cobalamin (vitamin B_{12}), pyrophosphate, flavin adenine dinucleotide (FAD), flavin mononucleotide (FMN), pyridoxal phosphate, coenzyme A, ascorbate (vitamin C), niacin, biotin, heme, porphyrin, folate, tetrahydrofolate, guanosine triphosphate, cytidine triphosphate, thymidine triphosphate, uridine triphosphate, retinol (vitamin A), calciferol (vitamin D_2), ubiquinone, ubiquitin, α-tocopherol (vitamin E), farnesyl, geranylgeranyl, pterin, pteridine or S-adenosyl methionine (SAM).

29. The method of claim 24, wherein said ligand is a nicotinamide adenine dinucleotide-related molecule.

30. The method of claim 29, wherein said nicotinamide adenine dinucleotide-related molecule is selected from the group consisting of oxidized nicotinamide adenine dinucleotide, reduced nicotinamide adenine dinucleotide, oxidized nicotinamide adenine dinucleotide phosphate, reduced nicotinamide adenine dinucleotide phosphate, and a mimetic thereof.

31. The method of claim 24, wherein said ligand is a adenosine phosphate-related molecule.

32. The method of claim 31, wherein said adenosine phosphate-related molecule is selected from the group consisting of adenosine triphosphate, adenosine diphosphate, adenosine monophosphate, and a mimetic thereof.

33. A method of modeling the three dimensional structure of a polypeptide, comprising the method of claim 24 followed by the step of:

(c) modeling the three dimensional structure of said polypeptide according to a structural model of said second member of said polypeptide pharmacofamily.

34. A method for constructing a ligand conformer model, comprising determining an average structure of the bound conformations of a ligand in a pharmacocluster.

35. The method of claim 34, wherein said ligand comprises a nicotinamide adenine dinucleotide-related molecule.

36. The method of claim 35, wherein said nicotinamide adenine dinucleotide-related molecule is selected from the group consisting of oxidized nicotinamide adenine dinucleotide, reduced nicotinamide adenine dinucleotide, oxidized nicotinamide adenine dinucleotide phosphate, reduced nicotinamide adenine dinucleotide phosphate, and a mimetic thereof.

37. A method for constructing a pharmacaphore model, comprising constructing a model that contains one or more selected conformation-dependent properties of one or more pharmacoclusters.

38. A method for identifying a binding compound for one or more members of a polypeptide pharmacofamily, comprising identifying a compound having a selected conformation-dependent property of a pharmacocluster.

39. A pharmacocluster selected from the group consisting of pharmacocluster 1, pharmacocluster 2, pharmacocluster 3, pharmacocluster 4, pharmacocluster 5, pharmacocluster 6, pharmacocluster 7, and pharmacocluster 8.

40. A polypeptide pharmacofamily, comprising polypeptides that bind to substantially the same bound conformation of a nicotinamide adenine dinucleotide-related molecule selected from pharmacofamily 1, pharmacofamily 2, pharmacofamily 3, pharmacofamily 4, pharmacofamily 5, pharmacofamily 6, pharmacofamily 7, and pharmacofamily 8.

41. A polypeptide pharmacofamily, comprising polypeptides that bind to a nicotinamide adenine dinucleotide-related molecule having a bound conformation selected from pharmacocluster 1, pharmacocluster 2, pharmacocluster 3, pharmacocluster 4, pharmacocluster 5, pharmacocluster 6, pharmacocluster 7, and pharmacocluster 8.

42. A ligand conformer model, comprising a ligand conformer model, selected from the group consisting of conformer model 1 having coordinates listed in Table 3C, conformer model 2 having coordinates listed in Table 4C, conformer model 3 having coordinates listed in Table 5C, conformer model 4 having coordinates listed in Table 6C, conformer model 5 having coordinates listed in Table 7C, conformer model 6 having coordinates listed in Table 8C, conformer model 7 having coordinates listed in Table 9C, and conformer model 8 having coordinates listed in Table 10C.

43. A moiety, comprising coordinates, selected from the group consisting of coordinates listed in Table 3C, coordinates listed in Table 4C, coordinates listed in Table 5C, coordinates listed in Table 6C, coordinates listed in Table 7C, coordinates listed in Table 8C, coordinates listed in Table 9C, and coordinates listed in Table 10C.

44. A pharmacophore model, comprising a pharmacophore model selected from the group consisting of pharmacophore model 1 having coordinates listed in Tables 3B and 3C, pharmacophore model 2 having coordinates listed in Tables 4B and 4C, pharmacophore model 3 having coordinates listed in Tables 5B and 5C, pharmacophore model 4 having coordinates listed in Tables 6B and 6C, pharmacophore model 5 having coordinates listed in Tables 7B and 7C, pharmacophore model 6 having coordinates listed in Tables 8B and 8C, pharmacophore model 7 having coordinates listed in Tables 9B and 9C, and pharmacophore model 8 having coordinates listed in Tables 10B and 10C.